

Properties of Many-polaron in Fractional Dimension Space

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Polaron binding energy and effective mass are calculated in the fractional-dimensional space approach using the second-order perturbation theory. The effect of carrier density on the static screening correction of the electron-phonon interaction is calculated using the Hubbard's local field factor. It is found that the effective mass and the binding energy both decrease with increase in doping.

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I. INTRODUCTION

When an electron in the bottom of the conduction band of a polar semiconductor moves, its Coulomb field displaces the positive and negative ions with respect to each other producing polarization field. The electron with the associated phonon cloud is known as a polaron[1]. The Fröhlich polaron results when the interaction between electron and longitudinal optic (LO) phonon is described in the Fröhlich form characterized by the dimensionless coupling constant α [2]. The polaron in an undoped polar material calculated with the unscreened electron-phonon interaction is termed as a single-polaron. In the weak coupling limit ($\alpha < 1$), the perturbation theory is applied to calculate ground state energies and effective masses of the single-polaron in three-dimensional (3D) polar materials[1], two-dimensional (2D) quantum well (QW) structures[3] and one-dimensional(1D) quantum wire structures[4].

When the width of the QW is extremely narrow and the barrier potential that causes the in-plane confinement is infinite, the system is purely 2D. The dimension increases monotonically with the increase of the well width and the infinitely wide well exhibits the three-dimensional (3D) behavior. In a finite QW with narrow well width, the electron envelope function spreads into the barrier region partially restoring the 3D characteristics of the system. The properties of the QW are determined by the parameters of the barrier materials. In the QW with large well width, the properties of the polaron are calculated taking the bulk values of the well material. This has been demonstrated in the calculation of exciton binding energy[5] and polaron properties as a function of well width[7]. Consequently, the QW with finite well width and barrier height shows fractional dimensional behavior with the dimension β lying between 2 and 3[6].

The anisotropic interactions in an anisotropic solid are treated as ones in an isotropic fractional dimensional space, where the dimension is determined by the degree of anisotropy[8]. Thus only a single parameter known as the degree of dimensionality β is needed to describe the system. The fractional dimensional space is not a vector space and the coordinates in this space are termed as *pseudocoordinates*[9].

The single-polaron binding energy and effective mass have been derived in rectangular and parabolic QWs[10]. When the carrier density is high, the electron-phonon interaction is dynamically screened by the frequency-dependent dielectric function and the resulting polaron is termed as the many-polaron. However, for systems with much larger plasma frequency than the LO phonon frequency, the static dielectric function can also be a good approximation. This happens when the carrier density is very large in the system. The properties of many-polaron in the doped ZnS was studied by da Costa and Studart[11] including the exchange-correlation effects beyond random phase approximation. They compared their results by including the Thomas-Fermi, Hubbard and more accurate static Slölander-Land-Tosi-Singwi (SLTS) local field factors. They found that the ground state energies and effective masses obtained with the Hubbard's local field correction are similar to those obtained in the SLTS method. We have therefore implemented the Hubbard's local field factor for calculating properties of the many-polaron.

II. POLARON BINDING ENERGY AND EFFECTIVE MASS

In the second-order perturbation method, the polaron binding energy is calculated from the electron self-energy due to electron-phonon interaction as[1]

$$E_{\beta D} = -\Sigma_{\beta D}(\mathbf{k}, \xi_k)|_{\mathbf{k}=0}, \quad (1)$$

where ξ_k is the electron energy with parabolic band dispersion ($\hbar^2 k^2 / 2m_b$). The effective mass in the same method is defined as

$$\frac{m_b}{m^*} = 1 + \left(\frac{m_b}{\hbar^2} \right) \frac{\partial^2 \Sigma_{\beta D}(\mathbf{k}, \xi_k)}{\partial k^2} \Big|_{\mathbf{k}=0} \quad (2)$$

where m_b is the band electron mass. The leading-order contribution to the electron self-energy due to the electron-phonon interaction at zero temperature is given by

$$\Sigma_{\beta}(k, \xi_{\mathbf{k}}) = \sum_q \frac{|M_{\beta}(q)|^2}{\epsilon_{\beta}^2(q, 0)} \left[\frac{1}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}} + \hbar\omega_{LO}} \right], \quad (3)$$

where ω_{LO} is the LO phonon frequency. Here $M_{\beta D}$ is the electron-phonon interaction in the Fröhlich form is given as

$$M_{\beta D}(q) = -i\hbar\omega_{LO} \left(\frac{(4\pi)^{\frac{\beta-1}{2}} \Gamma\left(\frac{\beta-1}{2}\right) R_p \alpha}{q^{\beta-1} \Omega_{\beta}} \right)^{\frac{1}{2}}, \quad (4)$$

where Γ is the Euler-gamma function and $R_p = \sqrt{\hbar/2m_b\omega_{LO}}$ is the polaron radius. The dimensionless coupling constant α is defined as

$$\alpha = \frac{e^2}{2\hbar\omega_{LO}R_p} \left(\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_0} \right), \quad (5)$$

where ϵ_0 and ϵ_{∞} are the static and high-frequency dielectric constants, respectively. The static dielectric function including the local-field factor is defined as

$$\epsilon_{\beta D}(q, rs) = \epsilon_{\infty} \left[\frac{1 - [1 - G_{\beta D}(q, rs)] V_{\beta D}(q) \chi_{\beta D}(q, rs)}{1 + G_{\beta D}(q, rs) V_{\beta}(q) \xi_{\beta D}(q, rs)} \right], \quad (6)$$

where $G_{\beta D}(q, rs)$ is the Hubbard local-field-factor given by

$$G_{\beta D}(q, rs) = \frac{1}{2} \frac{q^{\beta-1}}{(q^2 + k_F^2)^{\frac{\beta-1}{2}}}. \quad (7)$$

The dimensionless density parameter rs is given by

$$k_F r_s a_B = \left[2^{\beta-1} \Gamma^2 \left(1 + \frac{\beta}{2} \right) \right]^{\frac{1}{\beta}} \quad (8)$$

where a_B is Bohr atomic radius and k_F is Fermi wave vector.

The irreducible polarizability function $\xi_{\beta D}(q, rs)$ is defined as

$$\chi_{\beta D}^0(q, rs) = \sum_{\mathbf{k}} \frac{n_F(\mathbf{k} + \mathbf{q}) - n_F(\mathbf{k})}{\xi_{\mathbf{k}+\mathbf{q}} - \xi_{\mathbf{k}}}. \quad (9)$$

In the fractional dimensional method the sum over \mathbf{k} is transferred to integrating as

$$\sum_{\mathbf{k}} = \int_0^{\infty} k^{\beta-1} D J \int_0^{\pi} \sin^{\beta-1} \theta d\theta \quad (10)$$

Using Eq.(10) in Eq. (9), we find

$$\chi_{\beta D}^0(q, rs) = - \frac{2^{3-\beta} m_b k_F^{\beta}}{\pi^{\frac{\beta-1}{2}} \hbar^2 \beta q^2 \Gamma\left(\frac{\beta-1}{2}\right)} \int_0^{\pi} {}_2F_1\left(1, \frac{\beta}{2}; \frac{\beta+2}{2}; \frac{4k_F^2 \cos^2 \theta}{q^2}\right) \sin^{\beta-2} \theta d\theta, \quad (11)$$

where ${}_2F_1$ is the Gauss hypergeometric function.

The Fourier transform of e^2/r in the fractional dimensional space is obtained as

$$V_{\beta D}(q) = \frac{(4\pi)^{\frac{\beta-1}{2}} e^2 \Gamma\left(\frac{\beta-1}{2}\right)}{q^{\beta-1}} \quad (12)$$

Using Eqs. (6), (7), (10) and (12) in Eq. (1), the binding energy is obtained as

$$E_{\beta D} = -\alpha \hbar \omega_{LO} \frac{\Gamma\left(\frac{\beta}{2}\right)}{\sqrt{\pi} \Gamma\left(\frac{\beta}{2}\right)} \int_0^\infty \frac{dq}{\epsilon_\beta(q, r_s)(q^2 + 1)}. \quad (13)$$

Similarly the effective mass in Eq.(2) can be obtained as

$$\frac{m_b}{m^*} = 1 - 4\alpha \frac{\Gamma\left(\frac{\beta-1}{2}\right)}{\sqrt{\pi} \beta \Gamma\left(\frac{\beta}{2}\right)} \int_0^\infty \frac{q^2 dq}{\epsilon_{\beta D}^2(q, r_s)(q^2 + 1)^3}. \quad (14)$$

For nondegenerate systems ($rs \rightarrow \infty$), $\epsilon_{\beta D} = 1$. The integrals in above Eqs(11) and (12) can be analytically evaluated. Now The binding energy is derived as

$$E_{\beta D} = -\frac{1}{2} \alpha \hbar \omega_{LO} \frac{\sqrt{\pi} \Gamma\left(\frac{\beta-1}{2}\right)}{\Gamma\left(\frac{\beta}{2}\right)} \quad (15)$$

and the effective mass is given by

$$\frac{m^*}{m_b} = 1 - \frac{1}{4} \alpha \frac{\sqrt{\pi} \Gamma\left(\frac{\beta-1}{2}\right)}{\beta \Gamma\left(\frac{\beta}{2}\right)}, \quad (16)$$

III. RESULTS AND DISCUSSIONS

we have taken the several parameters of GaAs to calculate polaron properties. The band mass $m_b = 0.067 m_0$, where m_0 is the electron mass, $\epsilon_\infty = 13.18$ and $\epsilon_0 = 10.89$. The value of $\alpha = 0.03$ which is appropriate for calculating polaron properties in the weak coupling limit. The LO phonon energy ($\hbar \omega_{LO}$) is taken as 36.25 meV.

The binding energy and effective masses calculated for several r_s values for dimensions $\beta = 2, 2.5$ and 3 are shown in Table I. Both binding energies and effective masses are found to increase with the increasing r_s . This suggests that the polaron properties decrease with the increasing carrier density. This results due to screening of the electron-phonon interaction.

The polaron properties also decrease as the dimension decreases. As the dimension of the system decreases, the system becomes more confined. The confinement of the system decreases the physical properties.

Although the static Hubbard's local-field-factor for the screening of the electron-phonon interaction correctly predicts r_s and β dependence of the physical properties, it does not include the exchange and correlation effects properly. It is much higher than the dynamic local field factor as the later correctly includes the exchange and correlation effects. Therefore it is required that we calculate the dynamic local field factor using quantum version of the STLS method and screen the electron-phonon interaction term. The Matsubara frequency summation method is the right direction for achieving it. Such a work is in progress in our group.

r_s	Polaron Energy (eV)			Effective mass		
	$\beta = 2$	$\beta = 2.5$	$\beta = 3$	$\beta = 2$	$\beta = 2.5$	$\beta = 3$
0.001	0.416	0.296	0.210	1.120	1.067	1.041
0.01	0.417	0.315	0.255	1.121	1.070	1.047
0.10	0.424	0.325	0.272	1.123	1.071	1.049
1.0	0.430	0.328	0.274	1.124	1.072	1.050
10.0	0.430	0.340	0.275	1.125	1.073	1.051

Table I: Polaron binding energy shift and effective mass as a function of r_s for dimensions $\beta=2, 2.5$ and 3.

IV. CONCLUSIONS

In the present work the binding energy shift and effective mass of the many-polaron system are calculated in the fractional dimensional method by screening the electron-phonon interaction term. The exchange-correlation effects beyond the random phase approximation method is included in the Hubbard's method. The polaron properties are found to decrease with the carrier density.

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